HVAC&R Research
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/uhvc20

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Published online: 28 Feb 2011.

To cite this article: Jian Sun & T. Agami Reddy (2006) Calibration of Building Energy Simulation Programs Using the Analytic Optimization Approach (RP-1051), HVAC&R Research, 12:1, 177-196

To link to this article: http://dx.doi.org/10.1080/10789669.2006.10391173

Calibration of Building Energy Simulation Programs Using the Analytic Optimization Approach (RP-1051)

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Received February 5, 2005; accepted July 25, 2005

Reconciling results from detailed building energy simulation programs to measured data has always been recognized as essential in substantiating how well the simulation model represents the real building and its system. If the simulation results do not match actual monitored data, the programmer will typically "adjust" inputs and operating parameters on a trial-and-error basis until the program output matches the known data. This "fudging" process often results in the manipulation of a large number of variables, which may significantly decrease the credibility of the entire simulation. A major drawback to the widespread acceptance and credibility of the calibrated simulation approach is that it is highly dependent on the personal judgment of the analyst doing the calibration. The lack of a proper mathematical foundation for the general calibration problem has greatly contributed to the current state of affairs.

This paper proposes a general analytic framework for calibrating building energy system simulation software/programs that has a firm mathematical and statistical basis. The approach is based on the recognition that although calibration can be cast as an optimization problem, the basic issue is that the calibration problem is underdetermined or overparametrized, i.e., there are many more parameters to tune than can be supported by the monitored data. Further, detailed simulation programs are made up of nonlinear, implicit, and computationally demanding models. The proposed methodology involves several distinct concepts, namely, sensitivity analysis (to identify a subset of strong influential variables), identifiability analysis (to determine how many parameters of this subset can be tuned mathematically and which specific ones are the best candidates), numerical optimization (to determine the numerical values of this best subset of parameters), and uncertainty analysis (to deduce the range of variation of these parameters). A synthetic example involving an office building is used to illustrate the methodology with the DOE-2 simulation program. The proposed methodology is recommended for use as the second step of a two-stage process with the first being a coarse-grid search that has reduced the number of simulation input parameters to a manageable few and also narrowed their individual range of variability.

BACKGROUND AND OBJECTIVE

Standard building energy simulation programs typically produce electrical demand and consumption data as a program output. When calibrating such programs to existing buildings, the programmer will typically "adjust" inputs and operating parameters on a trial-and-error basis until the program output matches the measured data. This "fudging" process often results in the manipulation of a large number of variables, which may significantly decrease the credibility of

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the entire simulation (Troncoso 1997). Thus, the main reservations with the widespread use of calibrated simulation is that it is labor intensive and time consuming, requires a high level of user skill and knowledge in both simulation and practical building operation, and is highly dependent on the personal judgment of the analyst doing the calibration. The last reservation implies that this is more an art than a science and that, worse, the results are analyst-specific.

As a result, ASHRAE research project RP-1051 was initiated to provide systematic guidelines on how to calibrate detailed building energy simulation programs. The broad intent of that research was to cull the best tools, techniques, approaches, and procedures from the existing body of research and develop a coherent and systematic calibration methodology and a well-documented toolkit of robust procedures to help practicing energy engineers successfully reconcile computer simulations to measured data from actual buildings. The methodology developed, described, and illustrated in Reddy et al. (2006) essentially consists of four aspects: (1) define a set of influential input parameters and schedules along with their best-guess estimates and their range of variation depending on the building type, (2) perform a course grid search (involving hundreds of simulations) wherein the heuristically defined influential parameters are subject to a Monte Carlo simulation in order to identify a subset of the most sensitive parameters and to define narrower bounds of variability of such parameters, (3) perform a fine grid search to further refine the coarse grid search results by identifying a small set of feasible parameter vector solutions, and (4) use these solutions to determine the prediction uncertainty of the entire calibration process.

A detailed literature review of papers dealing with calibrated simulation of building energy simulation programs and allied issues has been published by Reddy (2006). Only a brief overview necessary for understanding of this paper is provided below. The calibration process adopted in the majority of studies involves tuning or refining the initial simulation input guess-values of the parameters in a heuristic manner that depends on the experience and expertise of the user. Clarke et al. (1993) classified the calibration into four broad types: (a) calibration based on manual, iterative, and pragmatic intervention (Diamond and Hunn 1981; Kaplan et al. 1990; Pedrini et al. 2002; Pedrini and Lamberts 2001; Yoon et al. 2003), (b) calibration based on a suite of informative graphical comparative displays (Bronson et al. 1992; Haberl et al.1993; Haberl and Bou-Saada 1998), (c) calibration based on special tests and analytical procedures (Soebarto 1997; Shonder et al. 1998; Manke and Hittle 1996; Liu et al. 2004), and (d) analytical/mathematical methods of calibration (Carroll and Hitchcock 1993).

The basic issue of the lack of a proper mathematical foundation to the calibration problem, however, remained unresolved, and it is this issue that this paper strives to address. The objective of this paper is, thus, to develop a methodology that contains the necessary elements for a more mathematical and statistical treatment of the calibration problem in general. More specifically, it is meant to enhance the capabilities of the fine-grid search described above in the framework of ASHRAE research project RP-1051 (Reddy et al. 2006). Toward this end, a rigorous analytical optimization methodology is proposed, described in mathematical terms, and illustrated by means of a case study.

DEVELOPMENT OF CONCEPT

The analytical/mathematical formulation of the calibration process proposed by Carroll and co-workers is closest in scope to the objectives of this study. It is akin to that of an optimization problem with the objective function being the minimization of the month-by-month (or even hour-by-hour if such data are available) mean square errors between measured and simulated energy use data. Such an approach, which would automatically determine which parameters to tune and by how much, has been formulated (Carroll and Hitchcock 1993) and developed to the extent that it was implemented in a commercially available, detailed simulation program called

RESEM (Carroll et al. 1989). The calibration problem is formulated as an unconstrained multi-objective problem termed *penalty function approach*, where the objective of minimizing the squared errors between measured and simulated energy use is combined with another term that tries to maintain reasonable values of the parameters **b** by adversely weighting the difference between the tuned parameters and their preferred or best-guess starting values. If the vector **b** denotes the set of *k* input parameters to be tuned, then the objective function is written as

$$\Delta_{m,n}(\mathbf{b}) = \sum_{i-1}^{m} w_i^{\delta}\delta_i^2 + \sum_{k=1}^{n} w_k^{\mathbf{b}}(\mathbf{b}_i - \hat{\mathbf{b}}_i)^2, \quad (1)$$

where δ is the difference between measured and simulated values of type of energy use *j* over *m* time scales (if utility bills over one year are used, $m = 12$ to represent one datum for each month of the year), w_i^{δ} is the weight (usually a fraction) associated with one particular type of energy use (say, electricity use or gas use) where one could change the weights to favor certain seasons of the year, and $w_k^{\mathbf{b}}$ is the weight associated with the penalty of deviating from the preferred values of the parameter set.

Note that the preferred vector $\hat{\mathbf{b}}$ is not necessarily the optimal solution of $\mathbf{b}^*$. Formulating the objective function in this manner is a simplification of the more rigorous approach of defining the objective function as the first term of Equation 1 and using the second term as a constraint. Solving a constrained optimization problem is more difficult than solving an unconstrained one, which is the reason why Carroll and Hitchcock adopted it. Standard gradient-based numerical techniques for finding optimal values of the parameter set **b** are then used during the calibration process.

Since numerical optimization is more efficient the fewer the parameters to be optimized, the authors suggest that the calibration process should first start with the process of reducing the number of parameters to be calibrated. This involves using sensitivity analyses to identify them. A recommendation is that this number be brought down to about 25 or less. The entire process was evaluated both using synthetic data from several prototypical buildings as well as from a limited sample of actual buildings. The authors also spell out various future enhancements to this work, such as using more matching criteria to the penalty function (e.g., including monthly demand data) and using knowledge-based system technology. On a final note, it must be mentioned that this procedure was developed for use with simplified simulation programs such as ASEAM (DOE 1991) and has not been used along with detailed fixed-step programs such as DOE-2 (Winkelmann et al. 1993).

Any general model being calibrated can be written as

$$\mathbf{j} = \mathbf{j}(\mathbf{v}, \mathbf{b}), \quad (2)$$

where

j = a vector of the simulated output, e.g., energy consumption and demand,
v = a vector of the measured input variables, and
b = a vector of the model parameters to be calibrated.

This model represents a system-level simulation that consists of a set of equations. Difference between the simulated outputs and the actual measured data can be quantified in a number of ways. The most common one is the least-squares method, which assumes that the best estimated parameters are the parameters that result in minimal sum of the deviations squared (*least-squares error*) between the simulated outputs and the actual measured data, also called residuals. Thus, the identification criterion (or the objective function) *J* is the sum of squares of

the model output residuals, which has to be minimized over the parameter vector **b**. With the weights set to unity (for the sake of simplicity), the minimization problem can be stated as

$$\min_{\mathbf{b}} \quad J = tr[\mathbf{r}^T(\mathbf{b})\mathbf{r}(\mathbf{b})] \tag{3}$$

$$\text{st.} \quad \mathbf{b}^{low} \le \mathbf{b} \le \mathbf{b}^{high},$$

where $tr(A)$ is the trace or the sum of the diagonal elements of the matrix A, **r** is the vector of model residuals, i.e., differences in the measured and predicted data points, and $\mathbf{b}^{low}$ and $\mathbf{b}^{high}$ denote the low and high values of the range of variability of **b**.

If the relative importance of each simulated output (for example, electric energy use and demand may have to be calibrated to different levels of accuracy) is to be explicitly factored in, a weight vector can be introduced in the identification criterion as described in Reddy et al. (2006). For solving such a weighted least-squares minimization problem, various optimization techniques can be used (Gill et al. 1981). Obviously, calibration of a detailed building simulation program/software is an overparameterized, nonlinear parameter estimation problem wherein it is impossible to try to identify all these parameters uniquely. The existence of non-unique solutions often results in a breakdown of such optimization algorithms. Therefore, a pretreatment procedure to identify the optimal parameter subset that can be best calibrated (and those that cannot be) is necessary. Flake (1998) addressed the parameter identifiability problem for models that can be written in explicit closed-form solution by checking the product of the derivative of the vector **j** with respect to parameter vector **b** as well as its variance-covariance matrix. In this study, a more systematic approach is proposed, which is more general in that it can be applied to any type of simulation model.

The analytical calibration process proposed involves four distinct processes: sensitivity analysis, identifiability analysis, optimization, and uncertainty analysis, as shown conceptually in Figure 1. Before the tuning process, represented as an optimization problem, can be reached, one has to perform both sensitivity and identifiability analyses. Sensitivity analysis allows the strong influential input parameters to be identified while the values of the weak variables are frozen at their default values without much adverse impact to the calibration process. Identifiability analysis is next used to find *how many* parameters and *which* parameters can be estimated uniquely based on available measured data (which could be utility bills only or utility bills supplemented with submetered and/or interval data). Finally, best guess-estimates of the uncertainty intervals of the unidentifiable parameters will be used in conjunction with a Monte Carlo analysis in order to determine the uncertainty in the tuned strong variables.

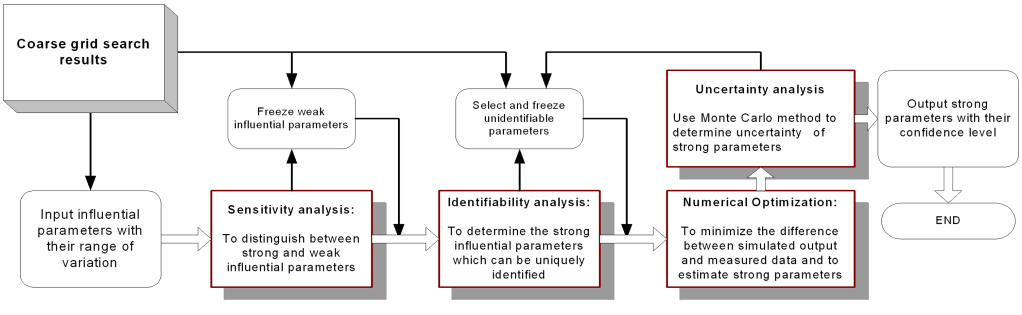

Figure 1. Flow chart depicting the various elements of the proposed analytical optimization approach.

SENSITIVITY ANALYSIS

Sensitivity analysis can be used for numerous purposes, as described by Reddy et al. (2006). In this study, the main purpose of sensitivity analysis is to distinguish the strongly influential parameters from the weakly influential parameters. Sensitivity coefficients (also called *elasticity* in economics as well as *influence* coefficients in thermal systems) are defined by the partial derivatives that indicate the magnitude of change of the response η due to perturbations in the values of the parameters **b**. For nonlinear systems, sensitivity coefficients will vary from point to point. Mathematically,

$$\mathbf{SC} = [sc_1 \; sc_2 \; \ldots \; sc_n] \text{ where } sc_k = \frac{\partial \mathbf{j}}{\partial \mathbf{b}_k} \qquad k = 1, 2 \ldots n \tag{4}$$

Sensitivity analysis involves selecting one or more simulated outputs (e.g., annual building energy consumption and/or demand) and determining which parameters influence these outputs significantly. Generally, there are three sensitivity analysis techniques (Lomas and Eppel 1992; Lam and Hui 1996): differential sensitivity analysis (DSA), random sensitivity analysis (RSA), and stochastic sensitivity analysis (SSA). DSA involves varying just one input for each simulation while the remaining input parameters are kept fixed. Several methods are available for evaluation of the sensitivity (Lomas and Eppel 1992): direction differential analysis, differential analysis by Green functions (or the variational method), differential analysis by finite differences (FD), approximate differential analysis, the polynomial approximation method, and differential analysis by automatic differentiation (AD). Among these methods, differential analysis by finite differences (FD) is most widely used because (1) it is easy to understand and calculate and (2) one derivative subroutine is easily applicable to any simulation program/software. One distinguishes between the following:

a. Individual sensitivity coefficients, which describe the sensitivity of the output due to variability in an individual input parameter:

$$sc_k = \frac{\partial \mathbf{j}}{\partial \mathbf{b}_k} = \frac{\Delta \mathbf{j}}{\Delta \mathbf{b}_k} = \frac{\mathbf{j} - \hat{\mathbf{j}}}{\mathbf{b}_k - \hat{\mathbf{b}}_k} \tag{5}$$

b. Total sensitivity coefficients, which describe the sensitivity of the output due to the combined variability of all the input parameters:

$$sc_{tot} = \left[\sum_{k=1}^{n} \left(\frac{\partial \mathbf{j}}{\partial \mathbf{b}_k} \right)^2 \right]^{1/2} = \left[\sum_{k=1}^{n} \left(\frac{\Delta \mathbf{j}}{\Delta \mathbf{b}_k} \right)^2 \right]^{1/2} = \left[\sum_{k=1}^{n} \left(\frac{\mathbf{j} - \hat{\mathbf{j}}}{\mathbf{b}_k - \hat{\mathbf{b}}_k} \right)^2 \right]^{1/2} \tag{6}$$

However, evaluating sensitivity coefficients by FD is not an attractive proposition. One of the reasons is the difficulty in selecting a reasonable finite difference interval to produce acceptable approximations. Improper choices often lead to poor results. There is no general procedure to guarantee it for every case. A standard choice is to select the interval that can minimize the total errors ε, which includes truncation error ε_t and round-off error ε_r. Barton (1992) investigated the method for choosing the forward difference interval and proposed a new dynamic interval size adjustment.

Another more serious disadvantage of finite difference estimation of sensitivity coefficients is the computation cost, particularly for simulation with a large number of independent variables. Normally, a gradient estimation requires numerous evaluations of the objective function. If the

simulation program/software has high nonlinearity and long run-times, the accuracy and computing cost will severely limit the finite difference approach from achieving acceptable results. An alternative approach, called *automatic differentiation* (AD) (Griewank 2000), has been suggested for use with building energy system simulation and optimization (Sun 2004; Sun and Reddy 2006). This is based on the mathematical concept of differential algebra, where the original function is decomposed into simpler elementary functions whose gradient vector and Hessian matrix are easy to find by applying first-order and second-order derivative calculations. The implementation is to repeatedly use the chain rule of elementary calculus but applied to floating point numerical values rather than to symbolic expressions. However, this algorithm has yet to be accepted, and it is not implemented in existing building energy simulation programs. For the illustrative case study, we have used the DOE-2 building energy simulation program (Winkelmann et al. 1993), which has yet to implement the AD algorithm. Hence, the simple perturbation method was applied to calculate the sensitivity coefficients given by Equation 4. Usually, the relative sensitivity coefficient is preferred.

$$sc_k = \frac{\partial \mathbf{j}}{\partial \mathbf{b}_k} \frac{\mathbf{b}_k}{\mathbf{j}} \tag{7}$$

In order to clearly indicate the influence of each parameter, we normalize the above sensitivity coefficient vector as

$$\mathbf{SC} = \left[\frac{sc_1}{\|\mathbf{SC}\|_2} \; \frac{sc_2}{\|\mathbf{SC}\|_2} \; \cdots \; \frac{sc_n}{\|\mathbf{SC}\|_2} \right], \tag{8}$$

where $\|\mathbf{SC}\|_2 = \sqrt{\mathbf{SC}^T \mathbf{SC}}$ is the Euclidean norm.

A sensitivity threshold value needs to be selected to distinguish parameters that can be considered to be strong and weak influential parameters. The choice of sensitivity threshold value is to some extent heuristic and is selected by the analyst.

IDENTIFIABILITY ANALYSIS

Mathematically, an identifiability analysis is defined as an investigation of the conditions under which parameters can be uniquely estimated (Beck and Arnold 1977). This is also the reason why it is regarded as a "uniqueness of solution" problem. If all the equations are linear, the problem is relatively simple since one can determine the rank of the matrix and thence infer the number of independent equations. However, if the equations are nonlinear, a more computer-intensive procedure is needed. As stated earlier, calibration is an overparametrized problem; only a subset of the parameters can be calibrated. Distinguishing this subset from other parameters will not only reduce the computational cost of the calibration process but also avoid the problem of numerical divergence during the optimization process. Identifiability analysis can achieve this objective by pre-analyzing a certain property of the system models. In this study, identifiability analysis will be considered as addressing two problems: (1) finding the number of identifiable parameters and (2) determining which parameters are best identified.

Mathematical Background to Find the Number of Identifiable Parameters

Any nonlinear, implicit system model can be written as

$$f(\mathbf{j},\mathbf{v},\mathbf{b}) = 0, \tag{9}$$

where **j** is a vector of the output, **v** is a vector of the measured input variables, and **b** is a vector of the input parameters to be calibrated.

Beck and Arnold (1977) presented an identifiability criterion to determine whether the parameters can be simultaneously estimated without ambiguity:

> Parameters can be estimated if the sensitivity coefficients over the range of the observation are not linearly dependent; i.e., the relation
>
> $$C_1\frac{\partial \mathbf{j}_i}{\partial \mathbf{b}_1} + C_2\frac{\partial \mathbf{j}_i}{\partial \mathbf{b}_2} + \ldots + C_n\frac{\partial \mathbf{j}_i}{\partial \mathbf{b}_n} = 0 \qquad (10)$$
>
> is true for all i observations and provided not all the C_k values are equal to zero. This is equivalent to stating that the matrix $[\frac{\partial \mathbf{j}}{\partial \mathbf{b}}]$ has full rank $\forall \mathbf{v}$.

This criterion can be easily applied to such systems where the sensitivity coefficients are explicit functions of input variables **v**. If such an explicit relation does not exist between sensitivity coefficients and input variables **v** (as is the case with detailed simulation programs), it is difficult to determine if the sensitivity coefficients over the range of the observation are linearly dependent or not. Thus, it is necessary to develop a general approach for determining the number of identifiable parameters from nonlinear equations, which is given below.

The popular methods (Beck and Arnold 1977) used for calibration are based on methods such as least squares, weighted least squares, and mean least estimation, all of which minimize the error between the measured data and model output following different criteria:

$$\text{Minimize } J = \Delta\mathbf{j}^T\mathbf{w}\Delta\mathbf{j} \qquad (11)$$

where J is the objective function, $\Delta\mathbf{j}$ is the vector of model residuals, and the weight matrix **w** is introduced to normalize for the numerical magnitude of the parameters **b**.

A Taylor series expansion of performance index J in the neighborhood of the local optima point $\mathbf{b}_0$ yields

$$I(\mathbf{b}) = J(\mathbf{b}_0) + \delta\mathbf{b}^T\nabla J(\mathbf{b}_0) + \frac{1}{2}\delta\mathbf{b}^T H(\mathbf{b}_0)\delta\mathbf{b} + HOT(|\delta\mathbf{b}|) \qquad \delta\mathbf{b} = \mathbf{b} - \mathbf{b}_0, \qquad (12)$$

where $\nabla J(\mathbf{b}_0) = \frac{\partial J(\mathbf{b}_0)}{\partial \mathbf{b}}$, $H(\mathbf{b}_0) = \frac{\partial^2 J(\mathbf{b}_0)}{\partial \mathbf{b}^2}$ is the Hessian matrix, and *HOT* denotes higher order terms.

The sufficient condition for a local minimum in the neighborhood of the point $\mathbf{b}_0$ is that the above Hessian matrix should be positive definite. The existence of a local minimum implies that we can find a set of values of parameters **b** by solving the above optimization problem. Interpreted in practical terms, this would imply that all the parameters **b** can be calibrated simultaneously. Determining whether the Hessian matrix is positive definite is difficult because second-order derivatives of the objective function need to be computed. A simplified approach involving first-order derivatives only is proposed below.

Consider the expression for the first-order derivative of the objective function:

$$\frac{\partial J(\mathbf{b}_0)}{\partial \mathbf{b}_k} = \left[\frac{\partial(\Delta\mathbf{j})}{\partial \mathbf{b}_k}\right]^T\mathbf{w}(\Delta\mathbf{j}) + (\Delta\mathbf{j})^T\mathbf{w}\frac{\partial(\Delta\mathbf{j})}{\partial \mathbf{b}_k} \qquad (13)$$

If **w** is assumed to be a square, symmetric, positive-definite matrix, then Equation 13 can be reexpressed as

$$\frac{\partial J(\mathbf{b}_0)}{\partial \mathbf{b}_k} = 2(\Delta\mathbf{j})^T\mathbf{w}\frac{\partial(\Delta\mathbf{j})}{\partial \mathbf{b}_k}. \qquad (14)$$

Recall that the Hessian of the input parameters to be calibrated is defined as follows:

$$H(\mathbf{b}_0) = \frac{\partial^2 J(\mathbf{b}_0)}{\partial \mathbf{b}^2} = \begin{bmatrix} J_{\mathbf{b}_1\mathbf{b}_1} & J_{\mathbf{b}_1\mathbf{b}_2} & & J_{\mathbf{b}_1\mathbf{b}_m} \\ J_{\mathbf{b}_2\mathbf{b}_1} & & & \vdots \\ & & J_{\mathbf{b}_k\mathbf{b}_l} & \ddots \\ J_{\mathbf{b}_m\mathbf{b}_1} & \cdots & & J_{\mathbf{b}_m\mathbf{b}_m} \end{bmatrix}. \tag{15a}$$

with

$$J_{\mathbf{b}_k\mathbf{b}_l} = \frac{\partial^2 J(\mathbf{b}_0)}{\partial \mathbf{b}_k \partial \mathbf{b}_l} = 2\left[\frac{\partial(\Delta \mathbf{j})}{\partial \mathbf{b}_l}\right]^T \mathbf{w} \frac{\partial(\Delta \mathbf{j})}{\partial \mathbf{b}_k} + 2(\Delta \mathbf{j})^T \mathbf{w} \frac{\partial^2(\Delta \mathbf{j})}{\partial \mathbf{b}_k \partial \mathbf{b}_l} \tag{15b}$$

(a) (b)

We assume the cross-derivative term (b) in the above equation to be negligible and define the weight as

$$w_{ij} = \begin{cases} w_i^2 & i = \mathbf{j} \\ 0 & i \neq \mathbf{j} \end{cases}. \tag{16}$$

Then Equation 15b simplifies into

$$J_{\mathbf{b}_k\mathbf{b}_l} = \frac{\partial J^2(\mathbf{b}_0)}{\partial \mathbf{b}_k \partial \mathbf{b}_l} = 2\left[\frac{\partial(\Delta \mathbf{j})}{\partial \mathbf{b}_l}\right]^T \mathbf{w} \frac{\partial(\Delta \mathbf{j})}{\partial \mathbf{b}_k} = 2\begin{pmatrix} a_k^1 & a_k^2 & \cdots & a_k^m \end{pmatrix} \begin{pmatrix} a_l^1 \\ a_l^2 \\ \vdots \\ a_l^m \end{pmatrix}, \tag{17}$$

where $a_k^i = w_i \frac{\partial \mathbf{j}_i}{\partial \mathbf{b}_k}$.

Usually, dimensionless sensitivity coefficients are used to replace those with dimensions. Then, one defines

$$a_k^i = w_i \frac{\partial \mathbf{j}_i}{\partial \mathbf{b}_k} \frac{\mathbf{b}_k}{\mathbf{j}_i} \tag{18}$$

and

$$\mathbf{s}_i = \begin{pmatrix} a_i^1 \\ a_i^2 \\ \vdots \\ a_i^n \end{pmatrix} i = 1, 2 \ldots m \tag{19}$$

from where Equation 17 can be rewritten as

$$J_{\mathbf{b}_k\mathbf{b}_l} = \frac{\partial J(\mathbf{b}_0)}{\partial \mathbf{b}_k \partial \mathbf{b}_l} = \mathbf{s}_k^T \mathbf{s}_l. \tag{20}$$

Let $\mathbf{S} = (\mathbf{s}_1\ \mathbf{s}_2\ ...\ \mathbf{s}_m)^T$. Then the simplified Hessian matrix, also called *identifiability matrix* or *correlation matrix* in this study, can be finally computed as

$$H(\mathbf{b}_0) = \frac{\partial^2 J(\mathbf{b}_0)}{\partial \mathbf{b}^2} = \mathbf{S}\mathbf{S}^T. \tag{21}$$

The Hessian matrix is a $(n \times n)$ square matrix. As previously, if $H(\mathbf{b}_0)$ is definite, all the n parameter variables are uniquely identifiable. Thus, we propose the following identifiability criterion:

> *The number of identifiable parameters is equal to the order of the highest order definite submatrix of the Hessian matrix. In other words, the rank of the Hessian matrix defines the number of uniquely identifiable parameters*.

Computing the rank of the Hessian matrix is much easier than checking whether the submatrix is positive definite or not. Theoretically, the rank of the Hessian matrix indicates the number of identifiable parameters. However, practically, even if a matrix is very close to singular, computer programs usually do not identify it as singular because of the high degree of their computational accuracy. Hence, a more robust method is to introduce the condition number that can indicate whether the Hessian matrix is ill conditioned or not. Then, the identifiability criterion can be recast as:

> *The number of identifiable parameters is equal to the order of the highest order definite submatrix (or the rank of the Hessian matrix) if the condition number of this submatrix is less than a predefined threshold valu*e.

The condition number of the identifiability matrix is well known and is defined by (Chatterjee and Price 1991)

$$\text{Cd} = \sqrt{\frac{\text{maximum eigenvalue of the correlation matrix}}{\text{minimum eigenvalue of the correlation matrix}}}. \tag{22}$$

The condition number indicates the collinearity of the parameters, with a large numerical absolute value representing strong collinearity. The correlation threshold is not based on any theoretical considerations but arises from empirical recommendations in the statistical literature. A value between 40 and 50 is often suggested as indicative of important collinearity between parameters (Ioslovich et al. 2004); this has been adopted in this study.

Mathematical Basis to Specify the Identifiable Parameters

The previous analysis provides an efficient method of determining the *number* of identifiable parameters but does not provide any insight on *which* parameters are best calibrated. This is the purpose of specifying the identifiable parameters. An approach based on analyzing the sensitivity and correlation coefficients is developed below that allows one to identify the most appropriate subset of parameters to calibrate.

With the given number of identifiable parameters, an obvious way is to select the parameters within the initial set that have high normalized sensitivity coefficients. Next, one could check the extent of their interdependence specified by the correlation coefficient. If all of them are uncorrelated or weakly correlated, they can be chosen as the parameter set to be identified. Otherwise, one has to remove the parameter with the lower sensitivity coefficient among the correlated pair, add another parameter with the next highest sensitivity coefficient among the remaining parameters of the identifiable parameter group, and repeat the process. In this man-

ner, the parameters that are uncorrelated and have relatively high sensitivity coefficients can be isolated from all the remaining parameters. The procedure is described in mathematical terms as follows.

First, normalize the residual vector $\mathbf{s}_j$ with their Euclidean norm, i.e.,

$$(\mathbf{s}_j)_N = \frac{\mathbf{s}_j}{\|\mathbf{s}_j\|_2} \tag{23}$$

where $\|\mathbf{s}_j\|_2 = \sqrt{\mathbf{s}_j^T \mathbf{s}_j}$ is the Euclidean norm. Then Equation 20 can be written as

$$J^N_{\mathbf{b}_k \mathbf{b}_l}(\mathbf{b}_0) = \left(\frac{\partial J(\mathbf{b}_0)}{\partial \mathbf{b}_k \partial \mathbf{b}_l}\right)_N = (\mathbf{s}_k)^T_N (\mathbf{s}_l)_N \tag{24}$$

and

$$\mathbf{S}_N = \left((\mathbf{s}_1)_N \, (\mathbf{s}_2)_N \, \ldots \, (\mathbf{s}_m)_N \right)^T.$$

Finally, the normalized Hessian matrix (normalized identifiability matrix) is given by

$$H_N(\mathbf{b}_0) = \left(\frac{\partial^2 J(\mathbf{b}_0)}{\partial \mathbf{b}^2}\right)_N = \mathbf{S}_N \mathbf{S}_N^T. \tag{25}$$

The diagonal elements of $H_N(\mathbf{b}_0)$ are equal to one, and the numerical values of the off-diagonal elements indicate the correlation coefficients of corresponding parameter pairs. If the absolute value of a pair is larger than a predefined threshold, then one of the parameters has to be dropped from the parameter set to be uniquely identified.

Implementation

Following the above analysis methodology, a general procedure for finding the identifiable parameters is summarized below.

1. Calculate the identifiability matrix given by Equation 21.
2. Check the rank, eigenvalues, and condition number of the identifiability matrix and determine the number of identifiable parameters.
3. Select an initial identifiable parameter set based on the strength of their sensitivity coefficients.
4. Calculate the normalized identifiability matrix by Equation 25.
5. Check the correlation coefficient of each pair of the initial set of identifiable parameters; if the correlation coefficient of a pair of identifiable parameters exceeds the preselected threshold, then remove the less sensitive one from the identifiable parameter pair. Add the next most sensitive unidentifiable parameter to this identifiable parameter group and repeat.

UNCERTAINTY ANALYSIS

From the previous analysis, the analytical optimization approach freezes the weakly influential parameters and unidentifiable strongly influential parameters at their default values, which are best-guess values set by the user. The calibrated results for identifiable strong parameters will be affected by the selection of these default values. The objective of the uncertainty analysis is to determine the uncertainty or range of variability associated with the identifiable strong parameters based on the uncertainty intervals of the weakly influential parameters and unidentifiable strongly influential parameters. In this study, the midpoint Latin Hypercube Monte Carlo (LHMC) algorithm (Reddy et al. 2006) is used to numerically determine the uncertainty of the

strong variables (any appropriate Monte Carlo variant could be used). For simplification, the uncertainty of the weak parameter can be neglected since the weak parameters have little or no influence on the calibrated results. The implementation of uncertainty analysis involves the following steps (Sun 2004):

1. Assume the unidentifiable strong parameters to have an uniform distribution within the given range (this is the simplest way, though any appropriate distribution can be assumed).
2. Discretize each of the unidentifiable strong parameters over the given range.
3. Generate midpoint LHMC combinations of these parameters.
4. With each combination, perform the calibration calculation to get the values of identifiable strong parameters.
5. Plot the distribution of the numerical values of the identifiable strong parameters and deduce appropriate statistics (mean, percentiles, etc.).

ILLUSTRATIVE EXAMPLE

A synthetic all-electric office building located in Philadelphia, Pennsylvania, is selected as the reference building, which is described fully by Reddy et al. (2006). The building energy simulation program DOE-2 is used as the simulation engine. A description of the building and systems is provided in Table 1. It is assumed that only the electric utility bills are known for one year, as shown in Figure 2. The "metered" electric energy use and demand values can be

Table 1. Description of Building and Systems Assumed for the Synthetic All-Electric Building (from Reddy et al. [2006])

Bldg. Type	Office	Units	Synthetic Building
General	Total size	ft^2/m^2	25,000/2323
	No. of stories		Single
	Dimensions (plane)	(ft × ft)/(m × m)	250 × 100/76 × 30.5
	No. of zones		5
Bldg. envelope	Roof		Construction 4 in. 70% abs 1 in. insulation
	Wall/window U-factor	$(Btu/°F·ft^2)/(kJ/K·m^2)$	0.175/1.1
	Wall U-factor	$(Btu/°F·ft^2)/(kJ/K·m^2)$	0.100/0.63
	Window U-factor	$(Btu/°F·ft^2)/(kJ/K·m^2)$	0.57/3.6
	Shading coefficient		0.75
	Lighting	$(W/ft^2)/(W/m^2)$	1.7/18.3
	Equipment	$(W/ft^2)/(W/m^2)$	1.0/10.8
	Occupant density		200 ft^2/person
Ventilation	Occupant/unoccupied		15/0 cfm/person
Thermostat setting	Occupied/unoccupied	°F/°C	72/22
Primary equipment			PVAV
Secondary equipment	Energy efficiency ratio		8
Heating	Electric heating		

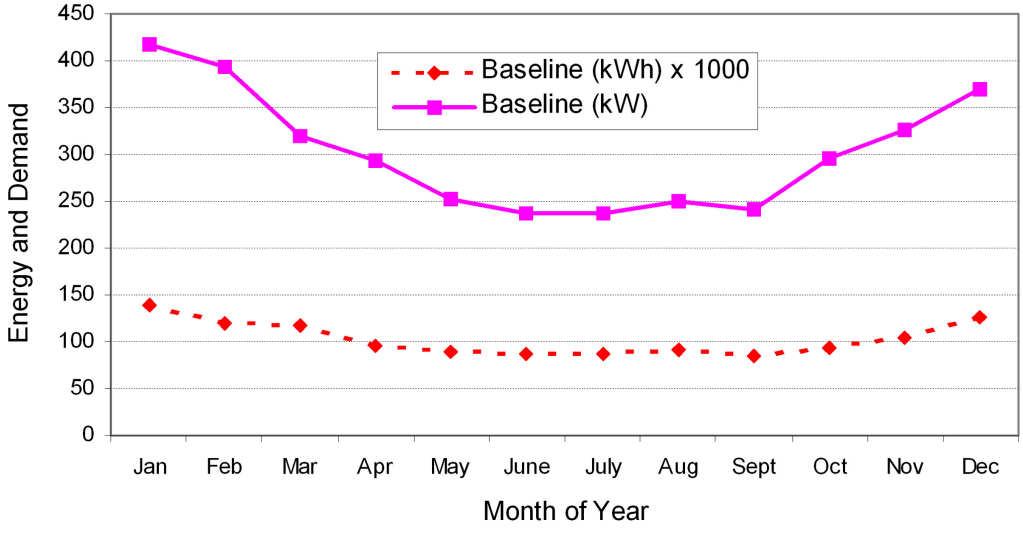

Figure 2. Time series plot of monthly electrical energy use and demand for synthetic all-electric building.

obtained by using the same simulation program engine under a well-defined input document in which input parameters have been assigned with reference values. During the calibrating process, input parameters will be adjusted so as to reduce the differences between the "metered" and monthly simulated energy use and demand (with both of them assumed to have the same weight factor, $w = 0.5$). The criterion is to check if the proposed analytical calibration procedure can tune or "recover" the input parameters back to the reference values.

Sensitivity Analysis

The parameters that need to be calibrated are listed in Table 2 following Reddy et al. (2006). These parameters are categorized into several groups as load schedules (which are vectors of 24 elements representing hourly diversity values for weekends and weekends and holidays separately), system schedules (which are vectors of 24 values representing hourly temperature settings), envelope loads, internal loads, system variables, and auxiliary electrical loads. As discussed above, the normalized sensitivity coefficients, determined by the perturbation method, have been calculated following Equation 8 and listed under the last column in Table 3. Selecting the threshold sensitivity coefficient as 0.15 (arbitrary but realistic), two groups of parameters can be easily defined depending on the numerical values of the normalized sensitivity coefficients: (a) seven strongly influential parameters (shown bold in Table 3) and (b) eight weakly influential parameters.

Identifiability Analysis

As stated previously, the weakly influential parameters are frozen at their default or reference values, as indicated in Table 3. Identifiability analysis is applied only to the strong parameters. In this study, we focus only on tuning the strong continuous parameters. At this time, a satisfactory procedure to tune the discrete parameters (such as diurnal schedules) has not been developed, and so this aspect is omitted in this study. Therefore, the identifiability matrix of the remaining six strong continuous parameters is computed following Equation 21, as shown in Table 4.

Table 2. List of Influential Parameters for the Typical Office Building Category (from Reddy et al. [2006])

	Description	Code	Variable Type*	Unit
Load schedules (rooms)	Lighting schedule	OffLgt	D	NA
	Equipment schedule	OffEqpt	D	NA
	Auxiliary equipment schedule	AuxEqpt	D	NA
Systems schedule (zones)	Space heating temperature schedule	OffHtT	D	NA
	Space cooling temperature schedule	OffClT	D	NA
Envelope loads	Window shading coeff.	SC	C	Fraction
	Window U-factor	Uwindow	C	Btu·h/°F·ft^2
	Wall U-factor	Uwall	C	Btu·h/°F·ft^2
Internal loads (rooms)	Lighting power density	LPD	C	W/ft^2
	Equipment power density	EPD	C	W/ft^2
Systems variables	Supply fan power/flow	SFP	C	kW/cfm
	Energy efficiency ratio	EIR	C	Fraction
	Minimum supply airflow	MinSA	C	Fraction
	Minimum outside air	MinOA	C	Fraction
Auxiliary electrical loads	Auxiliary electrical loads—non-HVAC effect	AuxElec	C	kW

*D—discrete, C—continuous.

Table 3. Range, Reference Values, and Normalized Sensitivity Coefficients of Input Parameters

Parameter	Unit	Minimum Value	Reference Value	Maximum Value	Normalized Sensitivity Coefficients
OffLgt	NA	OffLgt_1	OffLgt_D	OffLgt_2	0.0078
OffEqpt	NA	OffEqpt_1	OffEqpt_D	OffEqpt_2	0.0056
AuxEqpt	NA	AuxOffEqpt_1	AuxEqpt_D	AuxOffEqpt_2	0.0232
OffHtT	NA	OffHtT_1	OffHtT_D	OffHtT_2	**0.2966***
OffClT	NA	OffClT_1	OffClT_D	OffClT_2	0.0520
SC	Fraction	0.16	0.75	0.93	0.0512
Uwindow	Btu·h/°F·ft^2	0.25	0.57	1.22	0.0274
Uwall	Btu·h/°F·ft^2	0.055	0.64	0.8	**0.2280***
LPD	W/ft^2	1.3	1.7	2	0.0979
EPD	W/ft^2	0.8	1.0	1.2	0.0752
SFP	kW/cfm	0.001242	0.00145	0.001656	**0.1878***
EIR	Fraction	0.359	0.45	0.65	**0.3653***
MinSA	Fraction	0.3	0.65	1.0	**0.7420***
MinOA	Fraction	0.1	0.2	0.3	**0.1796***
AuxElec	kW	25	50	75	**0.2943***

* Strong parameters.
First five parameters are schedules.

Table 4. Identifiability Matrix or Unnormalized Hessian Matrix

	Uwall	SFP	EIR	MinSA	MinOA	AuxElec
Uwall	2.1984	2.7268	1.0833	1.8682	1.7023	1.8437
SFP	2.7268	8.9671	5.5755	6.8252	2.8428	8.2161
EIR	1.0833	5.5755	4.1134	4.2193	1.6027	5.3609
MinSA	1.8682	6.8252	4.2193	5.5854	2.0204	6.5339
MinOA	1.7023	2.8428	1.6027	2.0204	1.6444	2.1906
AuxElec	1.8437	8.2161	5.3609	6.5339	2.1906	7.9814

Table 5. Normalized Identifiability Matrix

	MinSA	EIR	AuxElec	Uwall	SFP	MinOA
MinSA	1	**0.88026**	0.97861	**0.53313**	0.96441	0.66668
EIR	0.88026	1	0.93561	**0.36024**	0.91802	0.61623
AuxElec	0.97861	0.93561	1	0.44015	0.97118	0.60467
Uwall	0.53313	0.36024	0.44015	1	0.61414	0.89534
SFP	0.96441	0.91802	0.97118	0.61414	1	0.74032
MinOA	0.66668	0.61623	0.60467	0.89534	0.74032	1

The rank of the previous identifiability matrix is 6 with the eigenvalues vector being

$$\lambda^6 = \left[0.0264\ 0.0366\ 0.1794\ 0.5997\ 2.4842\ 27.1637\right].$$

The condition numbers for this sixth-order matrix is

$$Cd^6 = 1028.93.$$

The same process is applied to the submatrix, and the eigenvalues and condition numbers are again computed. The maximum condition numbers of 5-order, 4-order, 3-order, and 2-order submatrices are calculated as shown below:

$$Cd^5 = 742.18, Cd^4 = 151.41, Cd^3 = 45.30, Cd^2 = 10.93$$

If the cutoff value is selected as 50, three of these condition numbers can be deemed too large. Thus, only three of the six strong continuous variables can be identified simultaneously. In order to determine which of these three identifiable parameters is best identified, the normalized identifiability matrix was calculated following Equation 25, and these parameters have been sorted from most to least sensitive based on their sensitivity coefficients (see Table 5).

The basic principle for selecting the identifiable parameters is to pick the most sensitive parameters that are not highly correlated with each other. As a start, three initial candidate identifiable parameters are selected as the three most sensitive parameters: MinSA, EIR, and AuxElec. Assume the threshold of the correlation coefficient to be 0.90. The correlation coefficient between MinSA and EIR is 0.88026, which is not sufficiently high to exclude EIR. However, parameters MinSA and AuxElec are strongly correlated (correlation coefficient equal to 0.98). Thus, the less sensitive one, AuxElec, is rejected from the candidate identifiable parameters list, and the next most sensitive parameter, namely, Uwall, is added to the candidate list. Hence, the final parameter set constituted of MinSA, EIR, and Uwall is deemed most suitable for selection as the identifiable parameter set.

Calibration Results

As described earlier, the numerical values of the three parameters are determined in the framework of an optimization problem. Specifically, a gradient-based nonlinear optimization technique has been used to find the numerical values of the calibrated parameters that minimize the coefficient of variation (CV) = (RMSE/annual mean) of the electricity energy use and demand residuals on a monthly basis, which are weighted equally. The iterative process is demonstrated in Figure 3, which shows the variation of three strong continuous identifiable parameters during the tuning process. Figure 4 indicates how the convergence characterized by the CV residual proceeds with iteration runs. These two figures indicate that the calibrated parameters reach their optimal tuning values after about 60 to 80 iterative simulation runs. The computation cost is acceptable for our engineering problem because each DOE-2 simulation run normally takes only a few seconds.

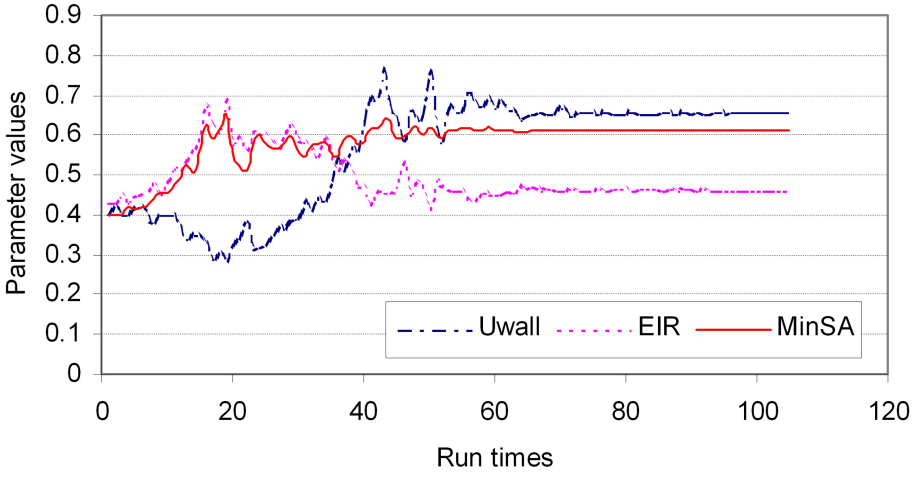

Figure 3. The variation of three continuous strong identifiable parameters with iterative runs during the tuning process.

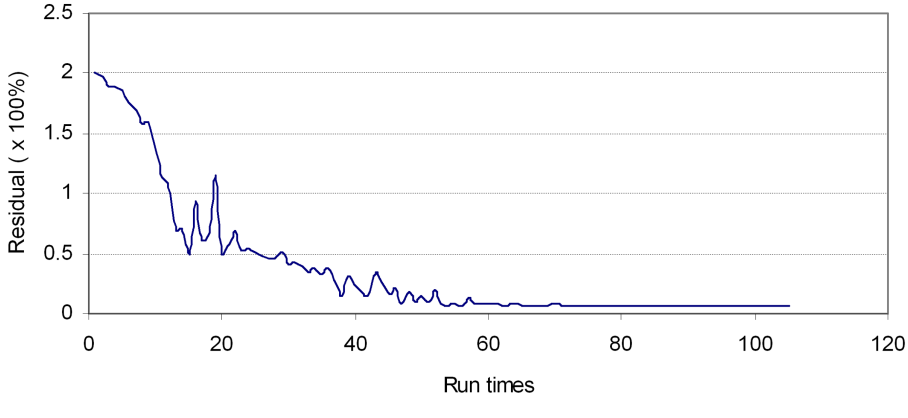

Figure 4. Convergence process of the CV residual with iterative runs during the tuning process.

The final results are shown in Table 6 and indicate that our calibration methodology is able to identify the parameters accurately. The reference values of the weak influential parameters and unidentifiable parameters are given in Table 2. Figure 5 shows how well our calibrated model is able to predict the "measured monthly electric energy use and demand." The mean monthly residual error is about 0.6%. This illustrative example demonstrates that the proposed analytical procedure, though involving several steps, is able to correctly tune the parameters back to their reference values.

Uncertainty of Calibration Results

The unidentifiable strong parameters were the Supply Fan Power/Delta_T (SFP), Minimum Outside Air (MinOA), and Auxiliary Electrical Loads—Non-HVAC effect. (AuxElec), which are assumed to be uniformly distributed over their uncertainty range, as specified in Table 3. According to the procedure described previously, the uncertainty distributions of the identifiable strong parameters were generated following the midpoint Latin Hypercube Monte Carlo (LHMC) algorithm and are shown in Figures 6 to 8. These figures lead to the following conclusions:

1. The median values of parameters MinSA, EIR, and Uwall are 0.64, 0.44, and 0.62, which agree well with their respective reference values of 0.65, 0.45, and 0.64. These are within 0.5%-2% of their respective reference values, thus indicating the accuracy of the proposed calibration methodology.

Table 6. Calibration Results

Identifiable Parameters	Reference Values	Low Bound	High Bound	Final Calibration Values	Initial Guess Values
Uwall	0.640	0.055	0.800	0.655	0.400
EIR	0.450	0.359	0.650	0.463	0.400
MinSA	0.650	0.300	1.000	0.612	0.400

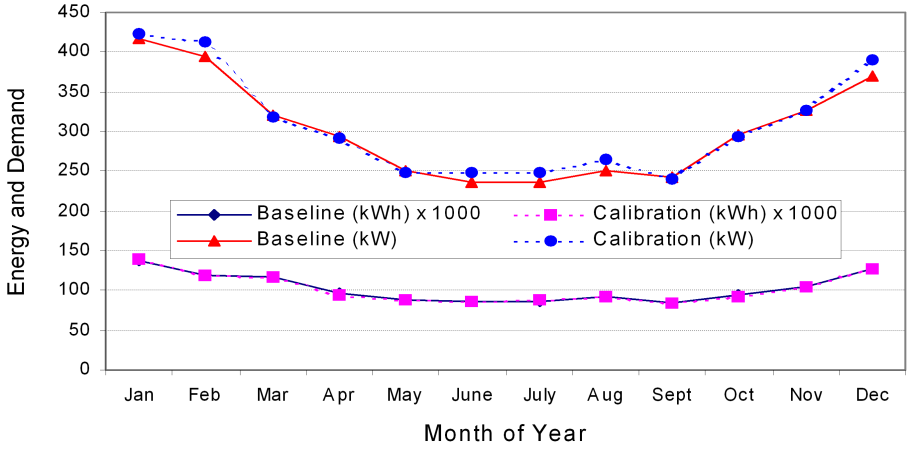

Figure 5. Plots illustrating how well our proposed analytical calibration method is able to predict measured monthly energy use and demand for the case study building.

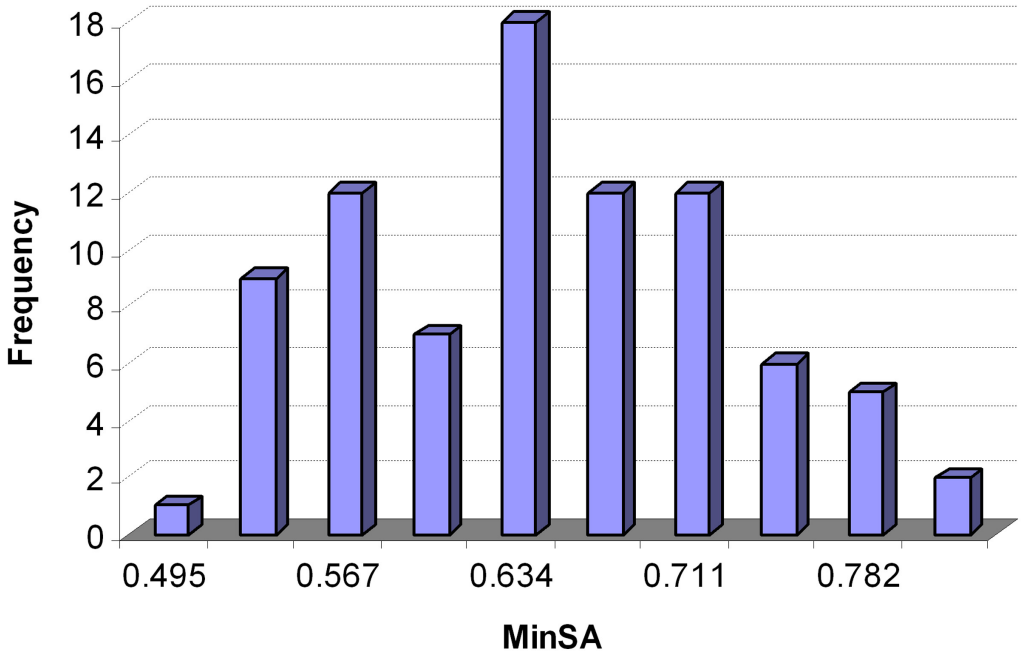

Figure 6. Uncertainty distribution of the calibrated variable MinSA whose reference value is 0.65.

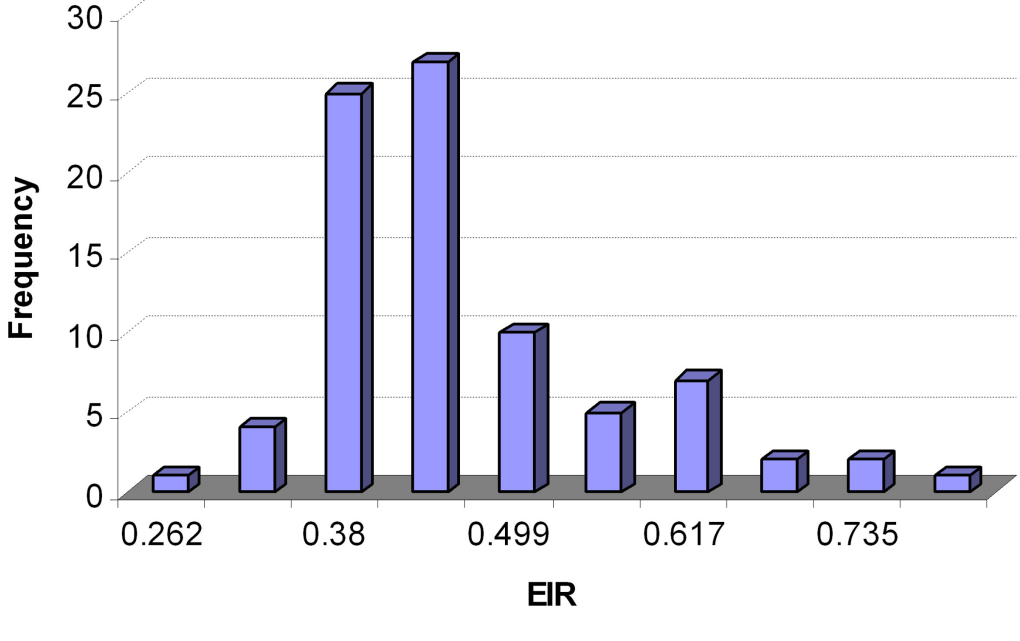

Figure 7. Uncertainty distribution of the calibrated variable EIR whose reference value is 0.45.

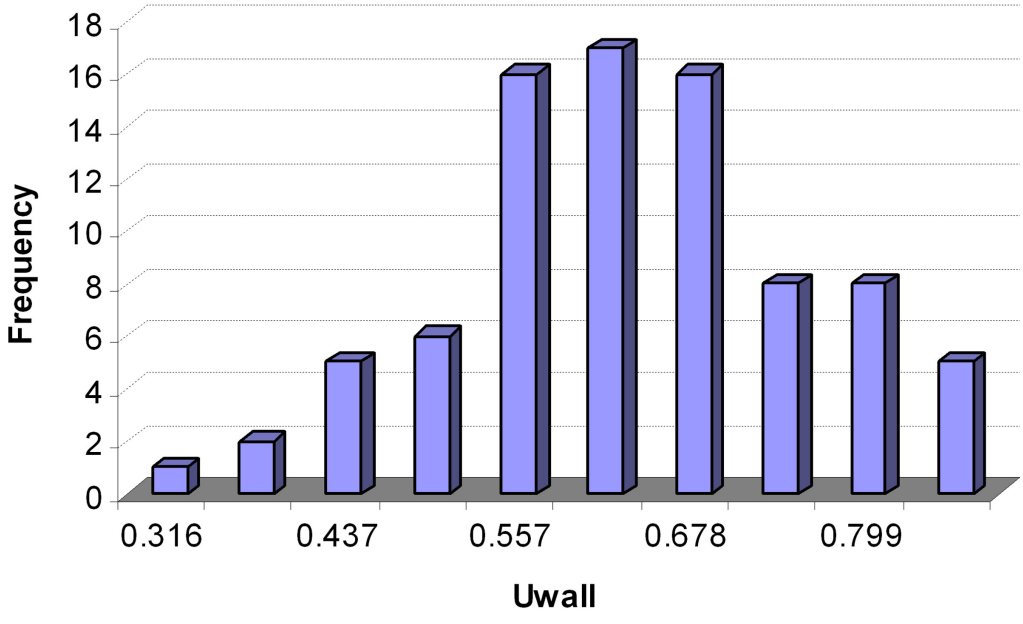

Figure 8. Uncertainty distribution of the calibrated variable Uwall whose reference value is 0.64.

2. The 90th percentile uncertainty intervals of the strong identifiable parameters MinSA, EIR, and Uwall are [0.53 0.78], [0.38, 0.62], and [0.44 0.8].
3. The parameter MinSA has relatively large uncertainty bands compared with EIR and Uwall. This indicates that the parameter MinSA is more easily affected by the default unidentifiable strong parameter than are parameters such as auxiliary electric loads EIR and Uwall.

SUMMARY AND FUTURE WORK

The intent of the present study was to formulate the general problem of calibrating building energy simulation programs in mathematical and statistical terms. Recognizing the fact that calibration of detailed building energy simulation programs is essentially a highly overparametrized (or underdetermined) problem that no amount of parameter "tweaking" can satisfactorily resolve, further compounded by the facts that the equations are nonlinear, implicit, and computationally intensive, we propose a four-step process to addressing this problem. Since this process is suitable only when the search region is relatively narrow, this procedure is best implemented as the second phase of a two-phase approach, with the first involving a coarse grid search through the parameter space, which narrows the search space (Reddy et al. 2006). The proposed methodology involves several distinct subelements, namely, sensitivity analysis (to identify a subset of strong influential variables), identifiability analysis (to determine how many parameters of this subset can be tuned mathematically and which specific ones are best candidates), numerical optimization (to determine the numerical values of this best subset of parameters), and uncertainty analysis (to deduce the range of variation of these parameters). A synthetic example involving an office building is finally used to illustrate the methodology with the DOE-2 simulation program. Different techniques than those adopted in this study could be used to tackle the four subelements into which the entire calibration problem has been divided.

Refinements of various aspects of the proposed methodology are worthwhile research problems, which may rekindle the interest of building energy scientists, engineers, and students in this important aspect of calibration of detailed building energy simulation programs and the energy conservation potential such an activity can engender.

NOMENCLATURE

a_i	= dimensionless weighted sensitivity coefficients (Equation 18)	**r**	= vector of model residuals
b	= vector of input parameters being calibrated	RMSE	= root mean square error
$\mathbf{b}_0$	= optimal or local minima values of **b**	**S**, **s**	= normalized sensitivity coefficients matrix, vector (Equation 19)
C	= constant parameters (Equation 10)	**SC**, **sc**	= sensitivity coefficient vector, element
Cd	= condition number (Equation 22)	tr	= trace or sum of the diagonal elements of the matrix
CV	= coefficient of variation	**v**	= vector of the measured input variables
H	= Hessian matrix	**w**	= weight matrix
j	= simulated output vector	w	= weight
J	= performance index (Equation 17)	λ	= eigenvalue
m	= total number of observations used for calibration	δ	= difference between measured and simulated values
n	= total number of parameters being calibrated		

Subscripts

i	= suffix for observation number, 1 ... m	N	= normalized
k, l	= suffix for model parameter being calibrated, 1 ... n		

Various other building physical parameters are defined in Table 2.

ACKNOWLEDGMENTS

This research was performed as part of an ASHRAE-funded research project (RP-1051) under Technical Committee 4.7. We would like to thank the PMSC members for their close supervision of this research. Valuable advice and assistance from Dr. I. Maor and Dr. C. Panjapornporn are greatly appreciated. Critical comments by Dr. D. Niebur, Dr. M. Piasecki, and Dr. J. Wen are also acknowledged.

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